Accelerating the parallel band edge state calculation of a semiconductor quantum dot

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Introduction

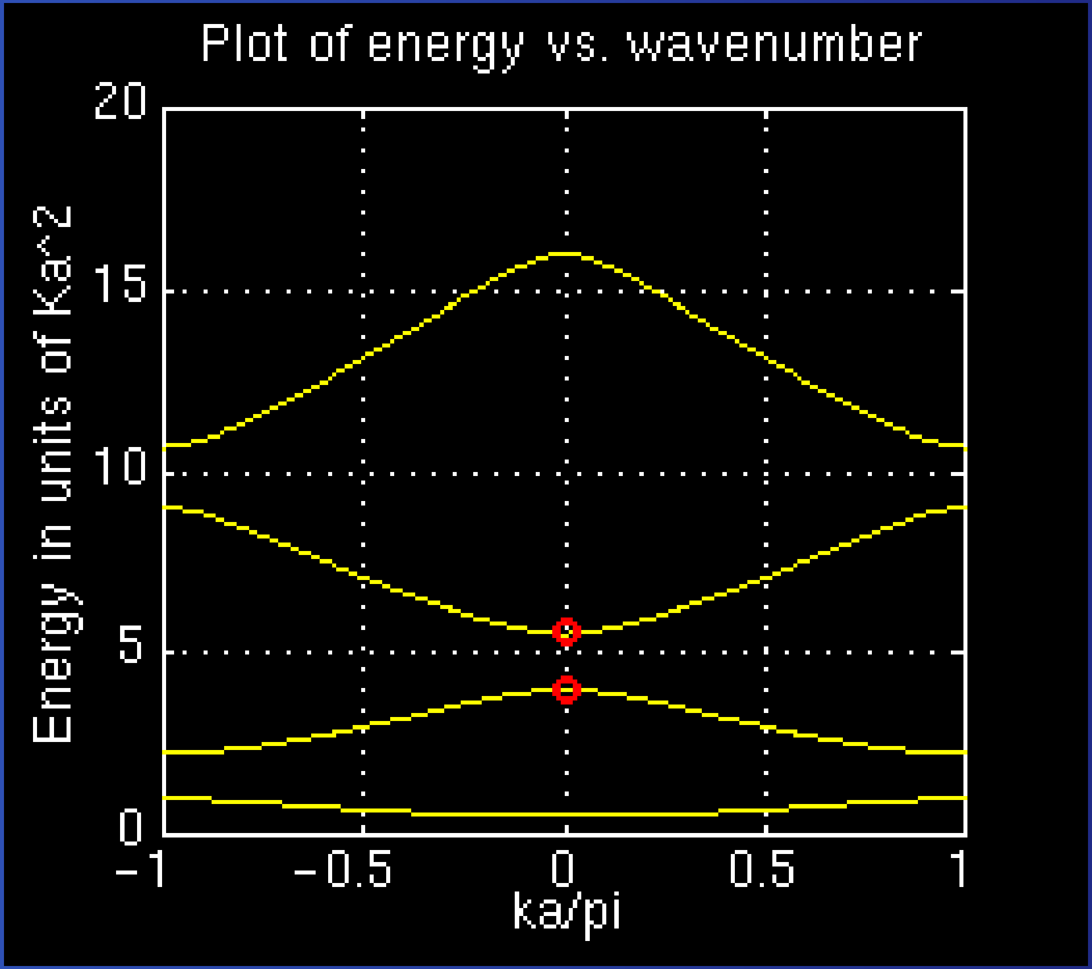
Computation of optical and electronic properties of materials

- Photo-luminescence

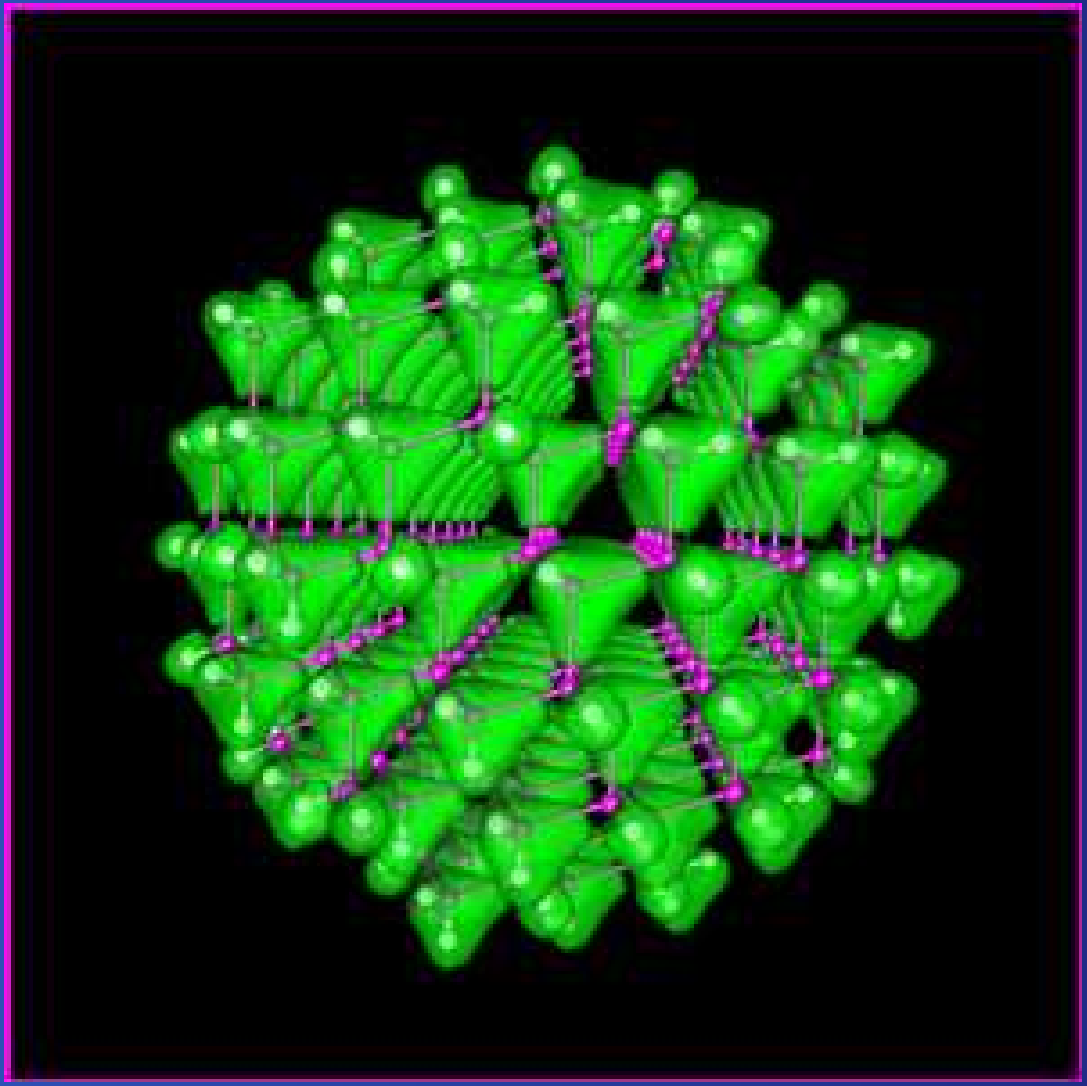
Two types of physical systems

- Crystals (*bulk*)
- Nanostructures, e.g. quantum dots

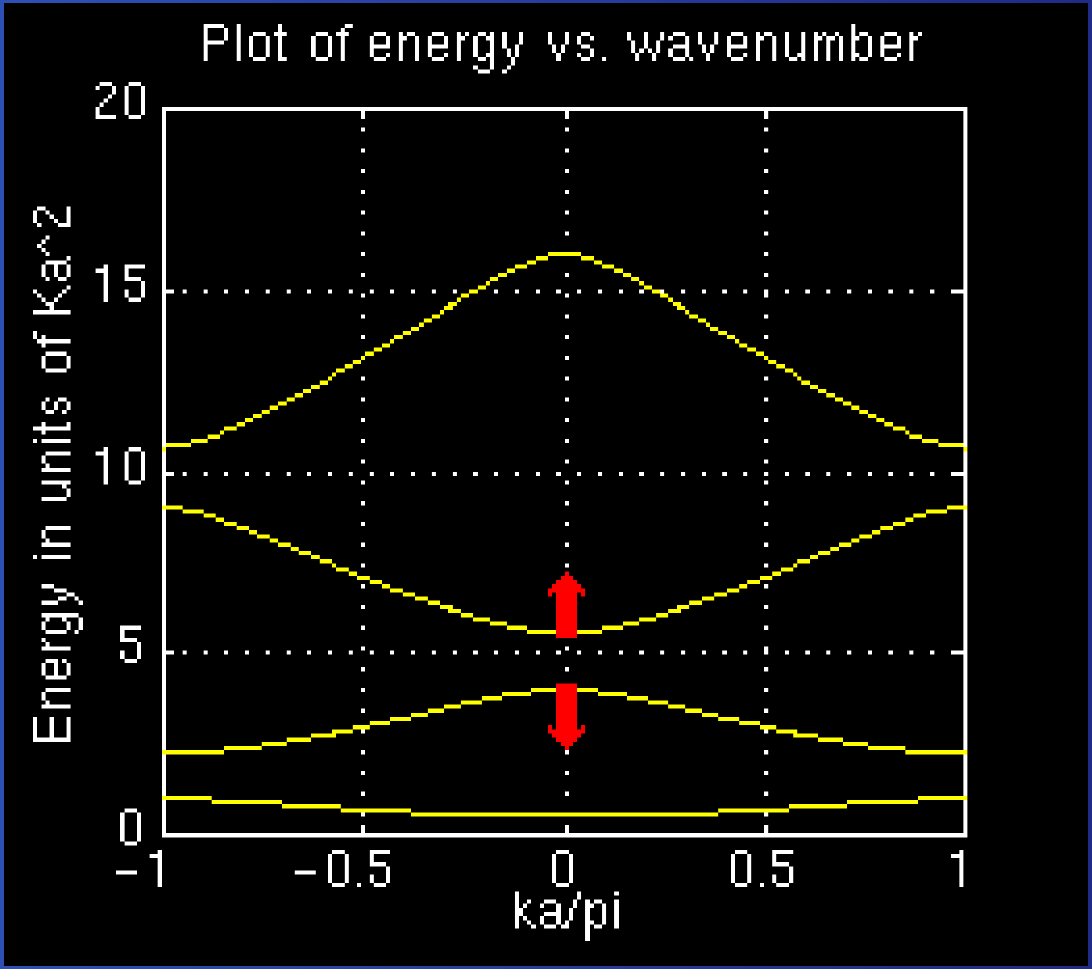
Infinite crystal: energy gap



Quantum dots



Quantum confinement effect



Approach

Observation: *qualitative* relationship between crystal and quantum dot states

Goal: *quantify* observation and *use* relationship for computations

Outline

- Schrödinger equation
- Subspace angles
- Preconditioned Conjugate Gradient
- Scalability issues
- Performance evaluation
- Summary

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- Computing resources: National Energy Research Scientific Computing Center

Schrödinger equation

Interior eigenvalue problem

$$H\Psi_i \equiv \left[-\frac{1}{2}\nabla^2 + V\right]\Psi_i = \epsilon_i \Psi_i,$$

Mathematical properties of *Hamiltonian* H

- Complex Hermitian indefinite
- Implicitly defined by MV product (uses FFT)
- Eigenvalues with higher multiplicities

Physical interpretation

Complex matrix $H = \left[-\frac{1}{2}\nabla^2 + V\right]$

- Laplacian ∇^2 corresponds to kinetic energy of electrons
- Potential V precomputed or from experiment

Real eigenvalue ϵ_i

- discrete energy level of electron
- can be occupied or unoccupied

Complex eigenvector Ψ_i

- probability distribution for spatial location (*state*) of electron

Subspace angles

Introduce S_{BB} (bulk band space)

- subset of eigenstates of crystal Hamiltonian
- subspace of ‘quantum dot space’
- of relatively small dimension
- thus cheaply computable
- sparse in plane wave basis
- *not* eigenstates of quantum dot

Projections

Orthogonal decomposition of quantum dot states:

$$\Psi_{QD} = \Psi_{BB} + \Psi_{BB^{\perp}}$$

Angle $\angle(\Psi_{QD}, \Psi_{BB})$ between state and its projection: $\approx 2^{\circ} - 3^{\circ}$ for examples shown later.

$\Rightarrow$ small, but not small enough.

Preconditioned Conjugate Gradient

For $A \equiv (H - E_{ref} I)^2$ find

$$\lambda = \text{arg} \min_{x \neq 0} \rho(x) \equiv \rho(x) = (x^H \; Ax)/(x^H x).$$

Residual $r_j \equiv Ax_j - \rho(x_j)x_j \parallel \nabla \rho(x_j)$

Given x_j, descent direction $d_j = -r_j + \beta_j d_{j-1}$, find

$$\theta_{j+1} = \text{arg} \min_{\theta} \rho(x_j \cos\theta + d_j \sin\theta).$$

$\Rightarrow$ x_{j+1} minimizes ρ in 2D subspace span $\{x_j, d_j\}$.

How to improve convergence of PCG

Starting vector: Find *cheap* x_0 such that $\rho(x_0)$ is as small as possible
$\Rightarrow$ use states from bulk as good approximations.

Preconditioner: Find *cheap* preconditioner P such that modified descent direction

$$d_j = -Pr_j + \beta_j d_{j-1},$$

reduces $\rho(x_0)$ as much as possible.

Details on preconditioner

Orthogonal decomposition of residual

$$r_{QD} = r_{BB} + r_{BB^\perp}$$

Additive preconditioner

$$P r_{QD} = P_{BB}\, r_{BB} + P_{BB^\perp}\, r_{BB^\perp}$$

P_{BB} from low-rank spectral approximation

$$(H_{BB} - E_{ref} I)^{-2} \approx \sum_{n,k} \Psi_{nk} (E_{nk} - E_{ref})^{-2}\, \Psi_{nk}^H$$

$\Rightarrow$ precondition projection of r_{QD} on S_{BB}.

Scalability issues

Efficient preconditioner implementation:

- Projection based on dot products of distributed vectors
- *Latency*-dominated runtime
- Solution: block communication to single blocked ALL_REDUCE

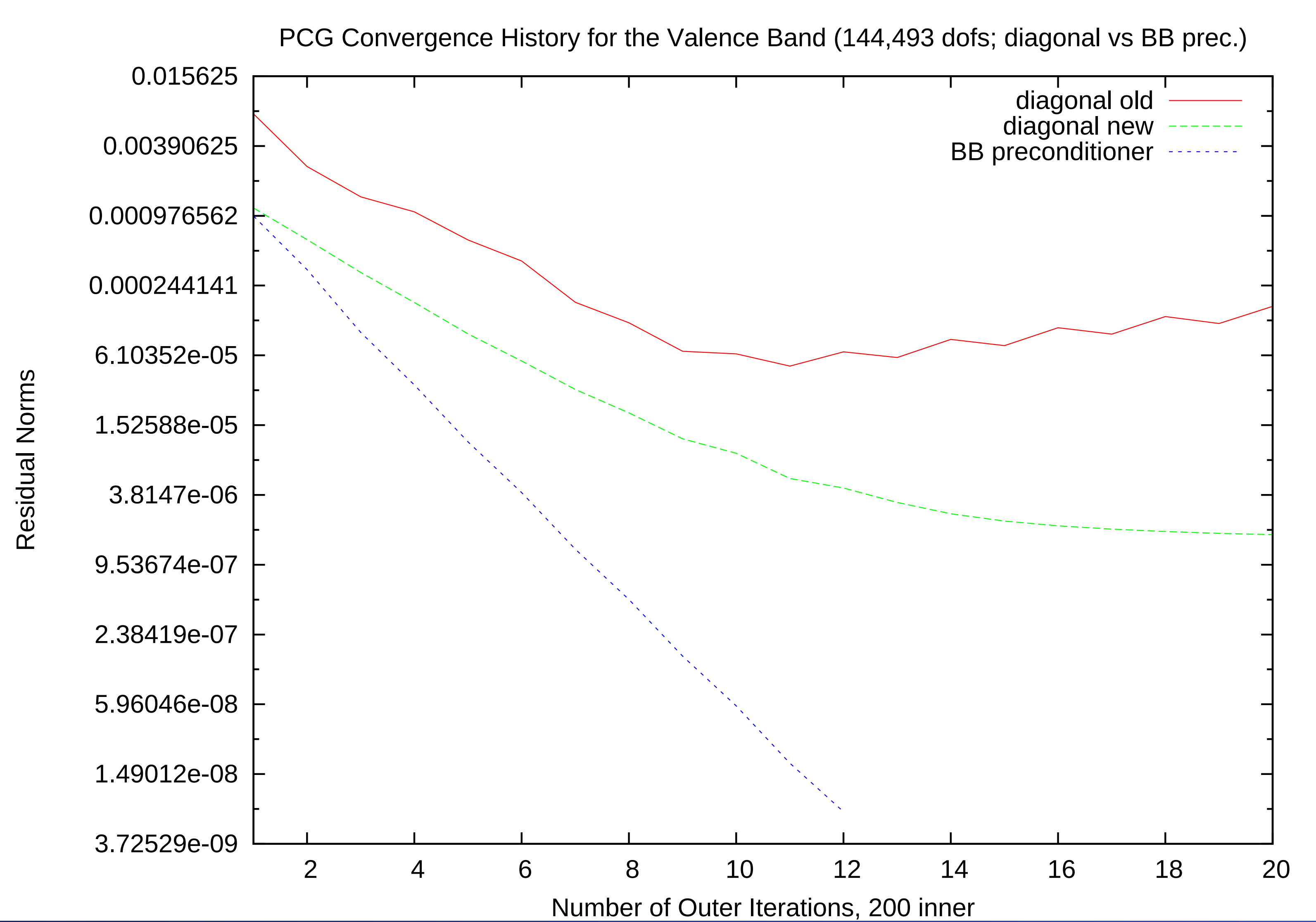
$\Rightarrow$ Cost increase per PCG iteration less than 5%.

Performance evaluation

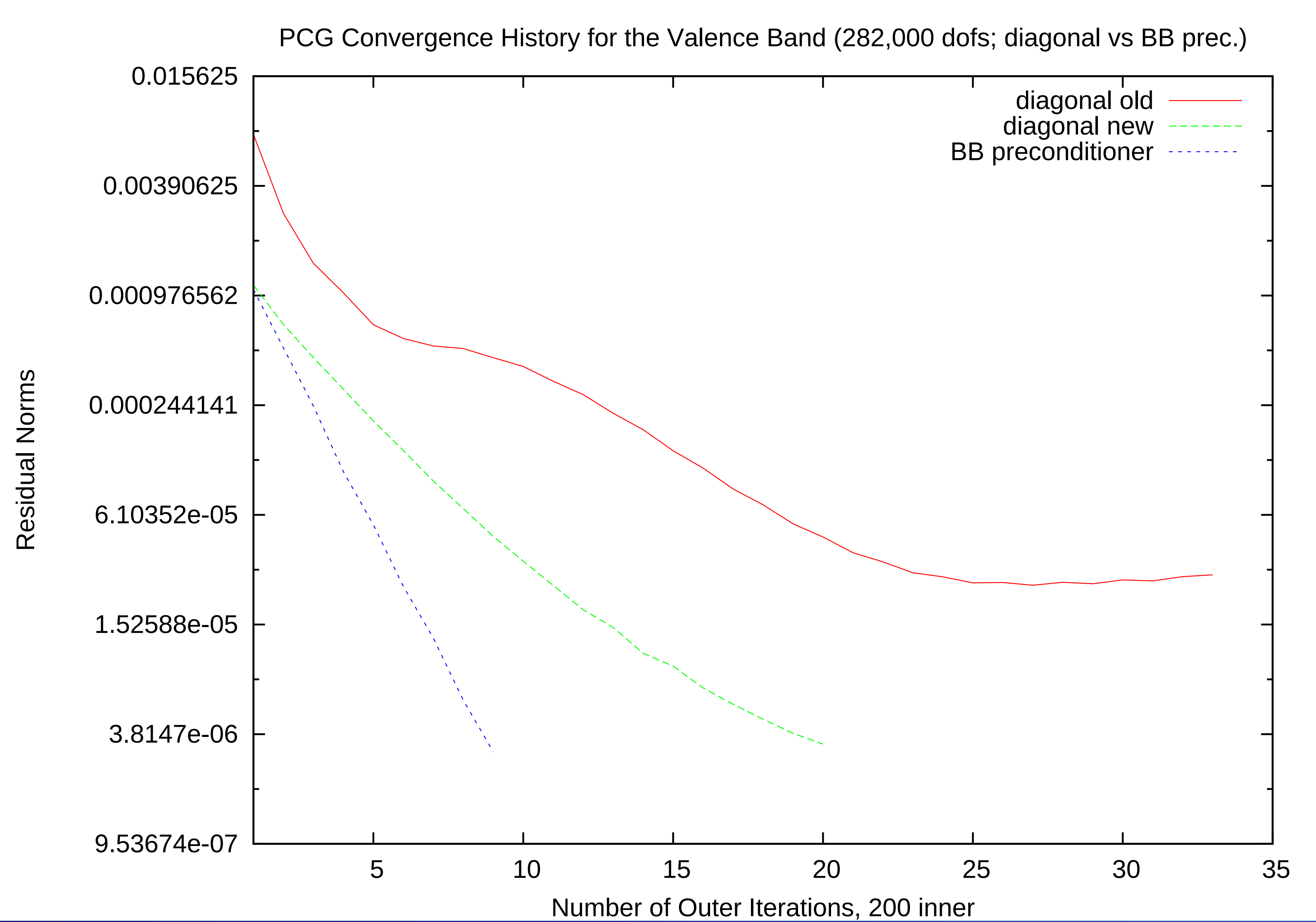
Quantum dot size (atoms)	system size (plane wave)	BB states (n,k)
784 Cd, 739 Se	145K	(5,949)
1568 Cd, 1601 Se	282K	(5,949)

Table 1: Test quantum dots. 16 processors, IBM SP.

QD1 (n=145K)


PCG Convergence History for the Valence Band (144,493 dofs; diagonal vs BB prec.)
Residual Norms
0.015625
0.00390625
0.000976562
0.000244141
6.10352e-05
1.52588e-05
3.8147e-06
9.53674e-07
2.38419e-07
5.96046e-08
1.49012e-08
3.72529e-09
2
4
6
8
10
12
14
16
18
20
Number of Outer Iterations, 200 inner
diagonal old
diagonal new
BB preconditioner

QD2 (n=282K)



PCG Convergence History for the Valence Band (282,000 dofs; diagonal vs BB prec.)
diagonal old
diagonal new
BB preconditioner
Residual Norms
0.015625
0.00390625
0.000976562
0.000244141
6.10352e-05
1.52588e-05
3.8147e-06
9.53674e-07
5
10
15
20
25
30
35
Number of Outer Iterations, 200 inner

Summary

- Crystal and quantum dot properties related: small angle between QD states and bulk subspace
- Accelerate convergence of PCG through improved initial vector and preconditioner, iterations decrease by at least factor of 3

Reference: *The use of bulk states to accelerate the band edge state calculation of a semiconductor quantum dot.* TR LBNL-60147, LBNL.